Modelling a turbulent reactive flow with variable equivalence ratio : Application to a flame stabilized by symmetrical backward-facing steps.

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Abstract

In this paper, an extension of the Bray-Moss-Libby model of turbulent combustion to reactive flows with variable equivalence ratio is presented and applied. The experimental configuration investigated¹ is a planar channel that incorporates a sudden expansion in a form of symmetrical backward-facing steps. As shown by Fig. 1, two lean mixtures of propane and air with different equivalence ratio are injected in the two halves of the entrance part of the channel, separated by a plate. In each stream, turbulence can be considered as fully developed at a distance x=-6h, where h is the height of a step. The numerical model includes a second-order closure for Reynolds stresses and uses a modified Bray-Moss-Libby model : BML ^{2,3,4,10} to take into account the influence of variable equivalence ratio. For the second order equations⁵, the different source terms are closed, using : the usual model of Launder et al. to model the pressure-rate of strain and the pressure-scalar correlations, the model due to Monin⁶ for Rotta's return to isotropy terms and the model due to Owen⁷ for the return to isotropy part of the production. Terms representing coupling between density inhomogeneities and the mean pressure gradient are expressed in a closed form by using the BML model. In the present work, two cases are investigated : in the first case, equivalence ratios of mixtures 1 and 2 are such that two oblique flames are obtained and merged downstream. In a second case, a single flame is obtained as the equivalence ratio of mixture 2 is smaller than the one corresponding to the lean extinction limit.



Figure 1: Experimental configuration

Combustion model

Assuming an isenthalpic flow with infinitely fast chemistry, we use the BML theory to express the mean production rate. In this approach, it is assumed that a turbulent premixed flame at large turbulent Damköhler number can be described as a statistical collection of infinitely thin laminar flamelets. The entire reative flow is then characterized by a bi-valued progress variable $c(x_i, t)$ which, in an isenthalpic configuration, can be identified to the reduced temperature. Assuming now that the Mach number of the reacting mixture is small, the pressure is supposed to be thermodynamically constant and the density variations are uniquely related to the temperature changes by way of the heat release parameter τ . Therefore the equation of state can be written as : $\bar{\rho} = \frac{\rho_R}{1 + \tau \tilde{c}}$ and the mean rate of chemical production \bar{w} , is expressed as :

$$\overline{w} = \rho_R U_L^o I^o \Sigma \tag{1}$$

 U_L^o is the burning velocity of an unstrained laminar flame, I^o is the mean quenching factor due to strain and curvature effects and Σ is the mean flamelet area per unit volume which can be related through an algebraic expression to the progress variable fluctuations and its integral length scale \hat{L}_y . The usual closure for I^{o8} assumed that local quenching may occur at scales smaller than the laminar flame thickness, that is, dissipative scales in the Kolmogorov energy spectrum. However, a theoretical study by Poinsot *et al*⁹ shows that these scales cannot quench the flame because their lifetimes are too short. Moreover, when the flamelet stretch is moderate, there is a flame surface production due to intermediate scales, leading to an increase in the mean chemical source term. Meneveau and Poinsot⁹ proposed a model for the stretch of the flame front by turbulent eddies (ITNFS model). Thus, the total flame stretch Γ_k is expressed as a function of L_t/δ_L with a very weak dependence on u'/U_L^o , where δ_L is the laminar flame front thickness :

$$\frac{U_L^o I^o}{\hat{L}_y} = \Gamma_k \frac{\tilde{\epsilon}}{\tilde{k}}.$$
(2)

Thermochemistry of reactive flow with variable equivalence ratio

The main objective of the present paper is to describe how equivalence ratio variations can be taken into account in an extended¹⁰ version of the BML model. Lahjaily *et al*¹⁰ consider the dilution of both products and fresh reactants by a surrounding air flow, in the case of a premixed stagnating turbulent flame. We take up this earlier extended version of the BML model to represent equivalence ratio variations within the flowfield. We define now the two states of the fuel-lean reactive flow : the unburnt mixture R is characterized by the absence of product species and the burnt gases Bcorresponding to the absence of propane. By introducing a classical mixture fraction f, wich is zero in the mixture 2 and unity in the mixture 1. Then, the state R(f) and B(f) are defined by :

$$Y_P^R = 0 \qquad Y_K^R = (Y_{K_2} - Y_{K_1})f + Y_{K_1} \qquad Y_{Ox}^R = 1 - Y_{K_1} + (Y_{K_1} - Y_{K_2})f$$

$$Y_K^B = 0 \qquad Y_P^B = Y_K^{st} / (Y_{K_2} - Y_{K_1})f + Y_{K_1} \qquad Y_{Ox}^B = Y_K^{st} / Y_K^{st} - (Y_{K_2} - Y_{K_1})f - Y_{K_1}$$

Where subscripts K, P and Ox stand for fuel, product species and air respectively and the subscripts 1, 2 and st stand for mixture 1 enter's conditions, mixture 2 enter's conditions and stoechiometric conditions respectively. The local instantaneous equivalence ratio can be simply expressed as : It is worth that B(f) represents both cases of undiluted and diluted burnt gases. Then, the change of state $R(f) \rightarrow B(f)$ is supposed to occur when $f > f_{min}$ where f_{min} corresponds to the lean-limit extinction of the fresh mixture R. A progress variable c and a mixture fraction f can be expressed as :

$$c(\underline{x}) = \frac{Y_P(\underline{x})}{Y_P^B(\underline{x})} \qquad f(\underline{x}) = \frac{Y_K(\underline{x}) - Y_{K1}}{Y_{K2} - Y_{K1}} + \frac{Y_K^{st} Y_P(\underline{x})}{Y_{K2} - Y_{K1}}$$

The expression for the fraction of fuel and product species as functions of c and f are given by :

$$Y_K = (1-c)(Y_{K_1} + f(Y_{K_2} - Y_{K_1}))$$
 and $Y_P = c f \frac{Y_{K_2} - Y_{K_1}}{Y_K^{st}} + c \frac{Y_{K_1}}{Y_K^{st}}$

The thermochemistry of the turbulent reactive flow is now completed by introducing a joint probability density function¹⁰ of f and c:

$$P(c, f, \underline{x}) = \alpha(\underline{x})\delta(c)P^{R}(f, \underline{x}) + \beta(\underline{x})\delta(1-c)P^{B}(f, \underline{x}) + \gamma(\underline{x})F(c, f, \underline{x})H(f - f_{min}) + \gamma_{m}(\underline{x})F_{m}(c, f, \underline{x})\left[1 - H(f - f_{min})\right]$$
(3)

 $P^{R}(f,\underline{x})$ and $P^{B}(f,\underline{x})$ represent the distributions of the mixture fraction in the fresh mixture and the burnt gases respectively and F and F_m are the distributions within the flamelets and within the non-reactive mixing zones between fresh mixture and burnt gases. The part of the pdf that corresponds to the non-reacive mixing between the reactants and products and then to a possible continuous variation of c between 0 and 1, is neglected, *i.e.*, $\gamma_m <<1$. The usual flamelet assumption is made *i.e.* combustion occurs only through infinitely thin interfaces, then $\gamma <<1$ and c is treated as a quasi-bivalued variable. Dilution effects are only including on terms $P^{R}(f,\underline{x})$ and $P^{B}(f,\underline{x})$. Using the expression of the joint pdf for c and f, the Reynolds averaged density and progress variable can be written as : $\overline{\rho} = \frac{\rho_R}{1 + \tau(f)\tilde{c}}$ where $\tau(f)$ is the mean heat release parameter. $\tau(f)$ is given by Metghalki and Keck¹¹ and is a non-linear expression of equivalence ratio $\phi = \phi(f)$. The mean production rate \overline{w} is expressed by the following relation :

$$\overline{w} = \gamma(\underline{x}) \int_0^1 \int_{fmin}^1 w(c, f) F(c, f, \underline{x}) dc df$$

Assuming that f and c are statistically independent and applying BML and ITNFS theory, we write \overline{w} as :

$$\overline{w} = \frac{g}{\sigma_y} \rho_R \frac{\widetilde{\epsilon}}{\widetilde{k}} \overline{c}(1-\overline{c}) \int_{fmin}^1 \Gamma_k P^R(f,\underline{x}) df = \frac{g}{\sigma_y} \rho_R \frac{\widetilde{\epsilon}}{\widetilde{k}} \overline{c}(1-\overline{c}) \widetilde{\Gamma_k}$$

Where $\widetilde{\Gamma_k}$ is the mean total stretch rate normalized by the large-scale strain. $\widetilde{\Gamma_k}$ depends on equivalence ratio via U_L^o and δ_L^{11} and is given by :

$$\widetilde{\Gamma_k} = \widetilde{\Gamma_k}[U_L^o(\phi), \delta_L(\phi)] = \frac{1}{\rho_R} \int_{fmin}^1 \rho_R \Gamma_k P^R(f, \underline{x}) df$$

Results and discussion

The resulting set of equations is solved on a rectilinear 2-D mesh by a finite-volume Navier-Stokes code ¹¹(Hadès) developed at the Laboratoire National d'Hydraulique of E.D.F. The two upstream flowfields are given from experimental data and assimilated to a flat velocity profil with common value $U_o = 20 m/s$. The inlet conditions for the velocity field are determined by a separate calculation of the isothermal turbulent flow developing in each half of the channel, using only the measured mean velocity of the flow. At the inlet *i.e.* x/h = -6, the mean progress variable c is set equal to 0 and the mixture fraction f is set equal to 1 and 0 for mixtures 1 and 2 respectively. To simulate ignition of the mixture, the mean progress variable is set to 0.85 in the kernels of the two recirculation zones. At the wall, the normal derivatives of Reynolds stresses components, progress variable and mixture fraction are assumed to be 0; the dissipation of turbulent kinetic energy $\tilde{\epsilon}$ is calculated through an equilibrium assumption between production and dissipation. Wall functions are used to provide boundary conditions for the mean velocity fields. In the present work two differents cases are investigated : in the first case, the equivalence ratios are $\phi = 0.9$, and $\phi = 0.3$ for mixture 1 and mixture 2 respectively ($\phi_{min} = 0.5$). In the second case, the equivalence ratios are $\phi = 0.9$, and $\phi = 0.7$ for mixture 1 and mixture 2 respectively. Numerical results are illustrated by figure 2 which gives two fields of mean chemical rate and two fields of mean temperature calculated for two differents sets of equivalence ratio. On a general point of view, the influence of the relative compositions of mixtures 1 and 2 on the mean structure of the flame zone is investigated. Fig. 2-b presents the field of mean temperature for the second case investigated : equivalence ratios of mixture 1 and 2 are 0.9 and 0.7 respectively ($\phi_{min} = 0.5$). Two oblique turbulent flames are stabilized by the two recirculation zones (0 < x/h < 5) downstream of the two symmetric steps. Within the two recirculation zones, there is an accumulation of hot products. Downstream of the recirculation zones, the flames merge in the region located between x/h = 12 and x/h = 20.



Figure 2: Fields of mean Temperature a) case 1, b) case 2, fields of mean reaction rate c) case1 and d) case 2.

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